

Likelihood ratio tests for positivity in polynomial regressions

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Abstract

A polynomial that is nonnegative over a given interval is called a positive polynomial. The set of such positive polynomials forms a closed convex cone K . In this paper, we consider the likelihood ratio test for the hypothesis of positivity that the estimand polynomial regression is a positive polynomial. By considering hierarchical hypotheses including the hypothesis of positivity, we define nested likelihood ratio tests, and derive their null distributions as mixtures of chi-square distributions by using the volume-of-tube method. The mixing probabilities are obtained by utilizing the parameterizations for the cone K and its dual provided in the framework of the Tchebycheff systems when the degree of polynomials is up to 4. Moreover, we propose the associated simultaneous confidence bound for polynomial regression curves. Regarding computation, we demonstrate that symmetric cone programming is useful to obtain the test statistics.

Key words: chi-bar square distribution, moment cone, positive polynomial cone, repeated measurements, symmetric cone programming, Tchebycheff system.

1 Introduction

Consider the polynomial regression model of degree n (≥ 1):

$$y_h = f(t_h; c) + \varepsilon_h, \quad f(t; c) = c^\top \psi(t) = \sum_{i=0}^n c_i t^i, \quad t \in T, \quad (1.1)$$

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$h = 1, \dots, N$, where $\psi(t) = \psi_n(t) = (1, t, \dots, t^n)^\top$ and $c = (c_0, c_1, \dots, c_n)^\top$ are column vectors in \mathbb{R}^{n+1} . The errors ε_h are independently distributed according to the normal distribution $N(0, \sigma^2)$ with mean 0 and variance σ^2 . $T \subseteq \mathbb{R}$ is the region of the explanatory variable t where the model (1.1) is defined. Typically, T is a bounded interval in \mathbb{R} . We assume that sufficient statistics of the model (1.1), that is, the ordinary least square estimator \hat{c} of c , and when σ^2 is unknown, the unbiased variance estimator $\hat{\sigma}^2$ of σ^2 distributed independently of \hat{c} are available.

In this paper, we deal with the hypothesis of positivity, or of superiority:

$$f(t; c) \geq 0 \quad \text{for all } t \in T. \quad (1.2)$$

To state its statistical meaning, it is natural to consider a two-sample problem. Let $f(t; c_{(j)}) = c_{(j)}^\top \psi(t)$ ($j = 0, 1$) be the polynomial regression curves of two groups. The hypothesis that the polynomial curve of group 1 is always bounded below by, or superior to, group 0 is expressed as $f(t; c_{(1)}) \geq f(t; c_{(0)})$ for all $t \in T$. Taking the difference, we see that (1.2) stands for the hypothesis of superiority. It is also possible to model the difference of two profiles (mean vectors) by a polynomial without modeling profile of each group (see Section 4.2). This notion of superiority is particularly important in statistical tests for assessing new drugs (Liu, et al. (2009)).

The set of coefficients c satisfying (1.2) forms a closed convex cone:

$$K = K_n = \{c \in \mathbb{R}^{n+1} \mid c^\top \psi(t) \geq 0, \forall t \in T\}. \quad (1.3)$$

This is referred to as the cone of positive polynomials (Barvinok (2002)). K is closed, since $K = \bigcap_{t \in T} \{c \mid c^\top \psi(t) \geq 0\}$ is the intersection of closed sets. The hypothesis (1.2) is rewritten as $c \in K$. Including this hypothesis, we consider the following hierarchical hypotheses:

$$H_0 : c = 0, \quad H_1 : c \in K_n, \quad \text{and} \quad H_2 : c \in \mathbb{R}^{n+1} \text{ (} c \text{ is unrestricted)}. \quad (1.4)$$

We then formalize the test for positivity as the likelihood ratio test (LRT) for testing H_1 against H_2 . In addition, we define an LRT for testing H_0 against H_1 . In the context of the two-sample problem, this is the test for the equality of two regression curves against the hypothesis of superiority. As we see later, it is mathematically convenient to treat the two LRTs at a time.

The theory of LRTs for convex cone hypotheses has been developed under the name of order restricted inference (Robertson, et al. (1988)). The general theorem states that the null distribution of LRT statistics is a finite mixture of chi-square distributions (Shapiro (1988)). When the cone has piecewise smooth boundaries,

Takemura and Kuriki (1997, 2002) proved that the weights (mixing probabilities) are expressed in terms of curvature measures on boundaries. This methodology is called the volume-of-tube method. Using this method, Kuriki and Takemura (2000) gave the weights associated with the cone of nonnegative definite matrices. However, the weights of few cones are obtained explicitly.

The main result of the present paper is the derivation of the weights associated with the cone of positive polynomials K , that is, the null distribution of the LRT for positivity. By applying the representation (parameterization) theorem for the positive polynomial cone and its dual cone developed in the framework of the Tchebycheff systems (Karlin and Studden (1966)), we evaluate the all weights of the two highest degrees (w_{n+1}, w_n) and the two lowest degrees (w_0, w_n) . In terms of these weights, the null distributions of the LRTs are expressed when the degree n of the polynomial regression is less than or equal to 4. When the degree n is more than 4, the upper and lower bounds for the null distributions are provided.

The outline of the paper is as follows. In Section 2, we present the expressions of the LRT statistics in both cases where the variance σ^2 is known and unknown. As in most statistical tests, we can also propose (simultaneous) confidence bands associated with the LRT for positivity. In Section 3, we first briefly summarize the volume-of-tube method. In order to apply this method, we need the volumes of the cone K , its dual cone, and their boundaries. Modifying the representation theorems for the positive polynomials in the Tchebycheff systems, we obtain explicit formulas for the weights. In Section 4, we discuss the computational aspects. To construct our LRT statistics, we need the maximum likelihood estimate (MLE) $f(t; \hat{c}_K)$, say, under the hypothesis of positivity. The coefficient \hat{c}_K is calculated as the orthogonal projection of \hat{c} onto the positive polynomial cone K . We show that this calculation can be conducted by symmetric cone programming, which is extensively studied in the optimization community. We also demonstrate an example of growth curve data analysis.

Throughout the paper, we treat only the polynomial regression. However, a polynomial is just one example of the Tchebycheff systems. The approach developed here is applicable to other systems. Another typical example is trigonometric regression

$$f(\theta; c) = c_0 + \sum_{i=1}^{n/2} \{c_{2i-1} \cos(i\theta) + c_{2i} \sin(i\theta)\}, \quad \theta \in \Theta \subseteq [0, 2\pi),$$

and we can consider the testing problem for the positivity once more. In this case, by changing a variable $t = \tan(\theta/2)$, all results in the polynomial regression are translated into the trigonometric regression.

2 Likelihood ratio tests and confidence bands

2.1 Likelihood ratio test statistics

Throughout the paper, we need to deal with a metric linear space and its dual space simultaneously. We write the inner product and the norm as

$$\langle x, y \rangle_Q = x^\top Q y, \quad \|x\|_Q = \sqrt{\langle x, x \rangle_Q},$$

where Q is a positive definite matrix. The orthogonal projection of x onto the set A with respect to the distance $\|\cdot\|_Q$ is denoted by

$$\Pi_Q(x|A) = \operatorname{argmin}_{y \in A} \|x - y\|_Q.$$

This is well defined when A is a closed convex set. The subscript Q in $\langle \cdot, \cdot \rangle_Q$, $\|\cdot\|_Q$, and Π_Q will be omitted when it does not cause any confusion.

In the regression model (1.1) with σ^2 known, the least square statistic \hat{c} is the sufficient statistic, and we can restrict our attention to the inference based on \hat{c} . The distribution of \hat{c} is the $(n+1)$ -dimensional normal distribution $N_{n+1}(c, \Sigma)$ with mean vector c and covariance matrix Σ , where $\Sigma = \sigma^2 \Sigma_0$ with $\Sigma_0 = (\sum_{i=1}^N \psi(t_i) \psi(t_i)^\top)^{-1}$, the inverse of the design matrix. When σ^2 is unknown, the sufficient statistic is the pair $(\hat{c}, \hat{\sigma}^2)$, where $\hat{\sigma}^2$ is the unbiased estimator of σ^2 calculated from the residuals, and is distributed proportionally to the chi-square distribution with $\nu = N - n - 1$ degrees of freedom.

Given the data \hat{c} distributed as the normal distribution $N_{n+1}(c, \Sigma)$ with $\Sigma = \sigma^2 \Sigma_0$ known, the MLE of c under the hypothesis of positivity $H_1 : c \in K$ is the orthogonal projection \hat{c}_K of \hat{c} onto the cone K under the metric $\langle \cdot, \cdot \rangle_{\Sigma^{-1}}$. When σ^2 is unknown, the MLE is the orthogonal projection onto K under the metric $\langle \cdot, \cdot \rangle_{\hat{\Sigma}^{-1}}$, $\hat{\Sigma} = \hat{\sigma}^2 \Sigma_0$. This MLE is the same as that with Σ known, because the orthogonal projection onto a cone is invariant with respect to the scale change of metric $\langle \cdot, \cdot \rangle_Q \mapsto \langle \cdot, \cdot \rangle_{kQ}$ ($k > 0$). The MLEs of c under H_0 and H_2 are given as 0 and \hat{c} , respectively. Acknowledging these facts, we obtain the LRT statistics as follows.

Proposition 2.1. *When the variance σ^2 is known, the LRT statistics for H_0 against H_1 , and for H_1 against H_2 are given by*

$$\lambda_{01} = \|\hat{c}_K\|_{\Sigma^{-1}}^2 \quad \text{and} \quad \lambda_{12} = \|\hat{c}\|_{\Sigma^{-1}}^2 - \|\hat{c}_K\|_{\Sigma^{-1}}^2, \quad (2.1)$$

respectively, where $\hat{c}_K = \Pi_{\Sigma^{-1}}(\hat{c}|K)$.

When the variance σ^2 is unknown and an independent and unbiased estimator $\hat{\sigma}^2$ of σ^2 with ν degrees of freedom is available, the LRT statistics for H_0 against H_1 , and for H_1 against H_2 are given by

$$\beta_{01} = \frac{\|\hat{c}_K\|_{\hat{\Sigma}^{-1}}^2}{\|\hat{c}\|_{\hat{\Sigma}^{-1}}^2 + \nu} \quad \text{and} \quad \beta_{12} = \frac{\|\hat{c}\|_{\hat{\Sigma}^{-1}}^2 - \|\hat{c}_K\|_{\hat{\Sigma}^{-1}}^2}{\|\hat{c}\|_{\hat{\Sigma}^{-1}}^2 - \|\hat{c}_K\|_{\hat{\Sigma}^{-1}}^2 + \nu}, \quad (2.2)$$

respectively, where $\hat{\Sigma} = \hat{\sigma}^2 \Sigma_0$, $\hat{c}_K = \Pi_{\hat{\Sigma}^{-1}}(\hat{c}|K)$.

The null hypotheses are rejected when the LRT statistics are greater than critical points.

The hypothesis of positivity H_1 is a composite hypothesis. To obtain the critical points for testing such a hypothesis, we need to know the least favorable configuration. The proof of the following proposition is essentially given in Section 2.3 of Robertson, et al. (1988).

Proposition 2.2. *In both cases where σ^2 is known or unknown, the least favorable configurations of the LRTs for testing H_1 (the hypothesis of positivity) against H_2 (the no-restriction hypothesis) are given by the case where H_0 holds, that is, $c = 0$.*

Proof. In the case where σ^2 is known, the acceptance region is of the form

$$A = \left\{ x \in \mathbb{R}^{n+1} \mid \min_{y \in K} \|x - y\| < d \right\}.$$

We first prove the monotonicity of the set A :

$$A - c = \{x - c \mid x \in A\} \supseteq A \quad \text{for any } c \in K.$$

This is because, for $c \in K$,

$$\begin{aligned} A - c &= \left\{ x - c \mid \min_{y \in K} \|x - y\| < d \right\} \\ &= \left\{ x \mid \min_{y \in K} \|x + c - y\| < d \right\} \\ &= \left\{ x \mid \min_{y \in K - c} \|x - y\| < d \right\} \supseteq \left\{ x \mid \min_{y \in K} \|x - y\| < d \right\} = A. \end{aligned}$$

The last inclusion follows from $K \subseteq K - c$, because K is a convex cone. Therefore, for $X \sim N_{n+1}(c, \Sigma)$,

$$\begin{aligned} P(X \in A \mid c) &= P(X + c \in A \mid c = 0) \\ &= P(X \in A - c \mid c = 0) \geq P(X \in A \mid c = 0), \end{aligned}$$

and $\inf_{H_1} P(X \in A \mid c) = P_{H_0}(X \in A)$ follows.

In the case where σ^2 is unknown, the LRT statistic β_{12} in (2.2) is rewritten as

$$\beta_{12} = \frac{\|\widehat{c}\|_{\Sigma^{-1}}^2 - \|\widehat{c}_K\|_{\Sigma^{-1}}^2}{\|\widehat{c}\|_{\Sigma^{-1}}^2 - \|\widehat{c}_K\|_{\Sigma^{-1}}^2 + \nu\widehat{\sigma}^2/\sigma^2} = \frac{\lambda_{12}}{\lambda_{12} + \nu\widehat{\sigma}^2/\sigma^2},$$

which is monotone in λ_{12} in (2.1). The monotonicity of the acceptance region can be proved similarly. \square

2.2 Simultaneous confidence bounds

In regression analysis, simultaneous confidence bounds for the estimated regression curve are often provided to assess the reliability of the estimated regression curve. The construction of confidence bands is still an active research topic because of its practical importance (Liu (2010)). In this subsection, we propose simultaneous confidence bands that are naturally linked to our proposed LRTs.

In general, when we want to construct simultaneous confidence bands for the regression curve $\{f(t; c) \mid t \in T\}$, we need to bound $|f(t; c) - f(t; \widehat{c})| = |(c - \widehat{c})^\top \psi(t)|$ above by a pivotal statistic whose distribution is independent of the true parameters. The most standard tool to obtain the upper bound is the Cauchy-Schwarz inequality. However, in this inequality, strict equality is attained when and only when (the closure of) the set of undirected rays spanned by the explanatory variable vectors $\{\alpha\psi(t) \mid t \in T, \alpha \in \mathbb{R}\}$ forms the whole space. In our polynomial regression model (1.1), this becomes the whole space \mathbb{R}^{n+1} only when $n = 1$ and $T = \mathbb{R}$ (Working and Hotelling (1929)). The cases where $n \geq 2$ or T is a proper subset of \mathbb{R} ($T \subsetneq \mathbb{R}$) are not easy problems and have been solved in limited cases (e.g., Uusipaikka (1983), Wynn and Bloomfield (1971)).

In our proposal, we relax the set of estimands from the regression curve itself. Let $\mu(dt)$ be a nonnegative measure on $T \subseteq \mathbb{R}$, and write $\mu[\psi] = \int_T \psi(t) \mu(dt)$. Then, $\mu[\psi] \in K^*$, where

$$K^* = K_n^* = \overline{\{\mu[\psi] \mid \mu(dt) \geq 0\}} \quad (2.3)$$

is the closure of the conic hull of the trajectory $\{\psi(t) \mid t \in T\}$. This cone is the dual cone of the positive polynomial cone K in (1.3), and is referred to as the moment cone (Barvinok (2002)). We construct the confidence bands on the basis of the inequality

$$\begin{aligned} \mu[f_{\widehat{c}}] - \mu[f_c] &= \int_T (\widehat{c} - c)^\top \psi(t) \mu(dt) = \langle \Sigma^{-1}(\widehat{c} - c), \mu[\psi] \rangle_\Sigma \\ &\leq \|\mu[\psi]\|_\Sigma \cdot \|\Pi_\Sigma(\Sigma^{-1}(\widehat{c} - c) | K^*)\|_\Sigma, \end{aligned} \quad (2.4)$$

where $\mu[f_c] = \int f(t; c) \mu(dt)$. The equality in (2.4) holds for some μ if and only if $\hat{c} - c \notin -K \setminus \{0\}$, where K is the positive polynomial cone in (1.3).

The statistics $\|\Pi_\Sigma(\Sigma^{-1}(\hat{c} - c)|K^*)\|_\Sigma$ in (2.4) is distributed independently of the true parameter c . Moreover, it is rewritten as

$$\begin{aligned} \|\Sigma^{-1}(\hat{c} - c)\|_\Sigma^2 - \min_{x \in K^*} \|\Sigma^{-1}(\hat{c} - c) - x\|_\Sigma^2 &= \|\hat{c} - c\|_{\Sigma^{-1}}^2 - \min_{y \in \Sigma K^*} \|\hat{c} - c - y\|_{\Sigma^{-1}}^2 \\ &= \|\Pi_{\Sigma^{-1}}(\hat{c} - c|\Sigma K^*)\|_{\Sigma^{-1}}^2 \\ &= \|\hat{c} - c\|_{\Sigma^{-1}}^2 - \|\Pi_{\Sigma^{-1}}(\hat{c} - c|K)\|_{\Sigma^{-1}}^2, \end{aligned}$$

which has the same distribution as λ_{12} in (2.1) under $H_0 : c = 0$. Using the upper α percentile $\lambda_{12,\alpha}$ of the distribution of λ_{12} under H_0 , we obtain the $1 - \alpha$ simultaneous confidence bands as follows.

Proposition 2.3. *The statement below holds with probability $1 - \alpha$:*

$$\mu[f_c] \in (\mu[f_{\hat{c}}] - \sqrt{\lambda_{12,\alpha}} \|\mu[\psi]\|_\Sigma, \infty) \quad \text{for all nonnegative measure } \mu \text{ on } T.$$

Considering a particular subclass of the nonnegative measures, we obtain various $1 - \alpha$ simultaneous confidence bands. For example,

$$f(t, c) \in (f(t, \hat{c}) - \sqrt{\lambda_{12,\alpha}} \|\psi(t)\|_\Sigma, \infty) \quad \text{for all } t \in T,$$

and

$$\int_{t_0}^t f(t, c) dt \in \left(\int_{t_0}^t f(t, \hat{c}) dt - \sqrt{\lambda_{12,\alpha}} \left\| \int_{t_0}^t \psi(t) dt \right\|_\Sigma, \infty \right) \quad \text{for all } t \in T$$

hold with probabilities more than or equal to $1 - \alpha$.

When σ^2 is unknown but its unbiased estimator $\hat{\sigma}^2$ with $\nu = N - n - 1$ degrees of freedom is available, we can obtain the simultaneous confidence bands by replacing $\|\cdot\|_\Sigma$ with $\|\cdot\|_{\hat{\Sigma}}$ ($\hat{\Sigma} = \hat{\sigma}^2 \Sigma_0$), and $\lambda_{12,\alpha}$ with $\lambda'_{12,\alpha}$, where $\lambda'_{12,\alpha}$ is the upper α quantile of the distribution of λ_{12}/\sqrt{s} , $s \sim \chi_\nu^2/\nu$.

3 Null distributions of the LRT statistics

3.1 The volume-of-tube method

In this subsection, we briefly summarize the volume-of-tube method.

Historically, the distributions of the orthogonal projection of a zero-mean Gaussian random vector have been well studied, since they appear as the null distribution of the test statistic in an order restricted inference. From the general

theory, the statistics λ_{01} and λ_{12} in (2.1) under the null hypothesis $H_0 : c = 0$ have the following distribution:

$$P_{H_0}(\lambda_{01} \geq a, \lambda_{12} \geq b) = \sum_{i=0}^{n+1} w_i \bar{G}_i(a) \bar{G}_{n+1-i}(b), \quad (3.1)$$

where \bar{G}_i is the upper probability of the chi-square distribution with i degrees of freedom. Note that $\bar{G}_0(a) = 1$ ($a < 0$), 0 ($a \geq 0$). In addition, the distribution of the LRTs β_{01} and β_{12} in (2.2) under H_0 is expressed as follows:

$$P_{H_0}(\beta_{01} \geq a, \beta_{12} \geq b) = \sum_{i=0}^{n+1} w_i \bar{B}_{\frac{i}{2}, \frac{n+1-i+\nu}{2}}(a) \bar{B}_{\frac{n+1-i}{2}, \frac{\nu}{2}}(b), \quad (3.2)$$

where $\bar{B}_{a,b}$ is the upper probability of the beta distribution with parameter (a, b) .

Note that the coefficients w_i appearing in (3.2) are the same as those in (3.1). They are nonnegative and satisfy $\sum_i w_i = 1$. This means that the distributions of $(\lambda_{01}, \lambda_{12})$ and (β_{01}, β_{12}) are finite mixture distributions with the same weights $\{w_i\}$. The marginal distributions of λ_{01} , λ_{12} , β_{01} , β_{12} can be obtained just by letting $a = -\infty$ or $b = -\infty$. The finite mixture distribution of the chi-square distributions in (3.1) is sometimes referred to as the chi-bar-square ($\bar{\chi}^2$) distribution (Robertson, et al. (1988), Shapiro (1988)).

When the cone K_n in (1.4) is polyhedral, that is, a finite intersection of half spaces, the weights $\{w_i\}$ can be understood in terms of the internal and external angles of each face of the cone (Wynn (1975)). Moreover, in the general case where K_n is not polyhedral, Takemura and Kuriki (1997, 2002) proved that the weights $\{w_i\}$ are expressed as integrals of elementary symmetric polynomials of principle curvatures of the boundaries of the cone K_n . These integrals are not easy to handle in general. However, the weights of the two highest degrees and two lowest degrees, w_{n+1}, w_n, w_0 and w_1 , have relatively simple expressions as follows:

$$\begin{aligned} w_{n+1} &= \frac{\text{Vol}_n(K \cap \mathbb{S}^n)}{\Omega_{n+1}}, & w_n &= \frac{\text{Vol}_{n-1}(\partial K \cap \mathbb{S}^n)}{2 \Omega_n}, \\ w_1 &= \frac{\text{Vol}_{n-1}^*(\partial K^* \cap (\mathbb{S}^n)^*)}{2 \Omega_n}, & w_0 &= \frac{\text{Vol}_n^*(K^* \cap (\mathbb{S}^n)^*)}{\Omega_{n+1}}, \end{aligned} \quad (3.3)$$

where ∂K and ∂K^* are the boundaries of K and K^* ,

$$\mathbb{S}^n = \{x \in \mathbb{R}^{n+1} \mid \|x\|_{\Sigma^{-1}} = 1\}, \quad (\mathbb{S}^n)^* = \{x \in \mathbb{R}^{n+1} \mid \|x\|_{\Sigma} = 1\}$$

are the unit spheres, Vol_d and Vol_d^* are d -dimensional volumes induced by the metrics $\langle \cdot, \cdot \rangle_{\Sigma^{-1}}$ and $\langle \cdot, \cdot \rangle_{\Sigma}$, respectively, and

$$\Omega_d = \frac{2\pi^{d/2}}{\Gamma(d/2)}$$

is the volume of the $(d-1)$ -dimensional unit sphere in \mathbb{R}^d . The lower dimensional measure is induced by the metric of the ambient space \mathbb{R}^{n+1} . It is also defined as the Hausdorff measure (Federer (1996)).

Moreover, a useful relation is known as a consequence of the Gauss-Bonnet theorem:

$$\sum_{i:\text{odd}} w_i = \sum_{i:\text{even}} w_i = \frac{1}{2}. \quad (3.4)$$

The distribution of β_{01} with $\nu = 0$ is interpreted as the volume formula of a spherical tubular neighborhood as below. Let $M = K \cap \mathbb{S}^n$ be the intersection of the cone K in (1.3) and the unit sphere. Define the spherical tube about M with the radius θ :

$$\text{Tube}(M, \theta) = \left\{ x \in \mathbb{S}^n \mid \min_{y \in M} \text{dist}(x, y) \leq \theta \right\}, \quad \text{dist}(x, y) = \cos^{-1} \langle x, y \rangle.$$

Then, because

$$\beta_{01} = \frac{\|\Pi(\hat{c}|K)\|^2}{\|\hat{c}\|^2} \geq \cos^2 \theta \Leftrightarrow \frac{\hat{c}}{\|\hat{c}\|} \in \text{Tube}(M, \theta),$$

and $\hat{c}/\|\hat{c}\|$ is distributed uniformly on \mathbb{S}^n under H_0 , we see that

$$\frac{\text{Vol}_n(\text{Tube}(M, \theta))}{\text{Vol}_n(\mathbb{S}^n)} = P_{H_0}(\beta_{01} \geq \cos^2 \theta) = \sum_{i=0}^{n+1} w_i \bar{B}_{\frac{i}{2}, \frac{n+1-i}{2}}(\cos^2 \theta).$$

This is the reason why our methodology is called the tube method.

The volume-of-tube method has been developed as a tool for approximating the tail probability of the maximum of a general Gaussian random field (Knowles and Siegmund (1989), Sun (1993), Adler and Taylor (2007)). This is regarded as a generalization of the distribution of the projection length of a Gaussian vector onto a convex cone (Kuriki and Takemura (2001)). This method is also used for the construction of confidence bands (Naiman (1990)). For the comprehensive survey, see Kuriki and Takemura (2009).

3.2 Representations for the cones K and K^*

In order to evaluate the volumes in (3.3), we need to introduce “local coordinates” of the cones K in (1.3), K^* in (2.3), and their boundaries ∂K and ∂K^* . This is actually possible by means of the representations in the theory of Tchebycheff systems. We consider the following three cases separately: (i) $T = [a, b]$ (bounded), (ii) $T = [a, \infty)$, and (iii) $T = (-\infty, \infty)$.

The two propositions below give presentations for the moment cone K_n^* and its boundary ∂K_n^* . Let

$$\psi_n(t) = \begin{cases} (1, t, \dots, t^n)^\top & (|t| < \infty), \\ (0, \dots, 0, (\pm 1)^n)^\top & (t = \pm \infty). \end{cases}$$

Let $\mathbb{R}_+ = (0, \infty)$, and

$$\Delta_m = \Delta_m(T) = \{\tau = (\tau_1, \dots, \tau_m) \in (\text{int } T)^m \mid \tau_1 < \dots < \tau_m\}. \quad (3.5)$$

Let $\Delta_0 = \emptyset$ formally.

Proposition 3.1. *The moment cone K_n^* on (i) $T = [a, b]$, (ii) $T = [a, \infty)$, or (iii) $T = (-\infty, \infty)$ (when $n = 2m$ is even) has the following almost sure representations. Let $a = -\infty$ when $T = (-\infty, \infty)$, and $b = \infty$ when $T = [a, \infty)$ or $(-\infty, \infty)$.*

$$\begin{aligned} K_n^* &= \phi_{n,n}^{(U)}\left(\mathbb{R}_+^{\lceil \frac{n+1}{2} \rceil + 1} \times \Delta_{\lfloor \frac{n}{2} \rfloor}\right) \\ &= \phi_{n,n}^{(L)}\left(\mathbb{R}_+^{\lfloor \frac{n}{2} \rfloor + 1} \times \Delta_{\lceil \frac{n+1}{2} \rceil}\right) \end{aligned} \quad (3.6)$$

almost surely with respect to the $(n+1)$ -dimensional Lebesgue measure, where

$$\phi_{n,l}^{(U)}(\rho, \tau) = \begin{cases} \sum_{i=1}^m \rho_i \psi_n(\tau_i) + \rho_{m+1} \psi_n(b) & (l = 2m), \\ \rho_1 \psi_n(a) + \sum_{i=1}^m \rho_{i+1} \psi_n(\tau_i) + \rho_{m+2} \psi_n(b) & (l = 2m+1), \end{cases} \quad (3.7)$$

and

$$\phi_{n,l}^{(L)}(\rho, \tau) = \begin{cases} \rho_1 \psi_n(a) + \sum_{i=1}^m \rho_{i+1} \psi_n(\tau_i) & (l = 2m), \\ \sum_{i=1}^{m+1} \rho_i \psi_n(\tau_i) & (l = 2m+1). \end{cases} \quad (3.8)$$

The maps $\phi_{n,n}^{(U)}$ and $\phi_{n,n}^{(L)}$ in (3.6) are diffeomorphic.

Remark 3.1. *The representations with (3.7) and (3.8) are called the upper and lower representations, respectively. They are coincident when $T = (-\infty, \infty)$ and $n = 2m$ (Definition 3.2 of Karlin and Studden (1966), Section 3 of Chapter II).*

Remark 3.2. *When $n = 1$, $\phi_{n,n}^{(U)}(\rho, \tau)$ is $\rho_1 \psi_1(a) + \rho_2 \psi_1(b)$, which does not contain the argument τ . In (3.6), $\phi_{n,n}^{(U)}(\mathbb{R}_+^{\lceil \frac{n+1}{2} \rceil + 1} \times \Delta_{\lfloor \frac{n}{2} \rfloor}) = \phi_{1,1}^{(U)}(\mathbb{R}_+^2 \times \emptyset)$ should read as $\{\phi_{1,1}^{(U)}(\rho, \tau) \mid \rho \in \mathbb{R}_+^2\}$. We use this convention in Propositions 3.1–3.4.*

Proof. The representations of the right-hand sides of (3.6) for $T = [a, b]$, $[a, \infty)$, and $(-\infty, \infty)$ are provided in Section 3 of Chapter II, Section 4 of Chapter V, and Section 2 of Chapter VI of Karlin and Studden (1966), respectively. The last case of $T = (-\infty, \infty)$ is stated in terms of periodic functions. Each of the upper and lower representations is the unique representation when $\rho_i > 0$ for all i , and all of a , τ_i and b are distinct.

Although the representations given by Karlin and Studden (1966) include the cases where $\rho_i = 0$ for some i , and some of a , τ_i and b take the same value, we can ignore them because the images of the maps $\phi_{n,n}^{(U)}$ and $\phi_{n,n}^{(L)}$ in such cases are $(n-1)$ -dimensional.

The maps $\phi_{n,n}^{(U)}$ and $\phi_{n,n}^{(L)}$ are one-to-one and obviously differential, that is, diffeomorphic. \square

Proposition 3.2. *Suppose that $n \geq 2$. Let Δ_m be defined in (3.5). Let $\phi_{n,l}^{(U)}$ and $\phi_{n,l}^{(L)}$ be defined in (3.7) and (3.8). The boundary of the moment cone ∂K_n^* has the following almost sure representation. Let again $a = \inf T$ and $b = \sup T$.*

(i), (ii) *When $T = [a, b]$ or $[a, \infty)$,*

$$\begin{aligned} \partial K_n^* = & \phi_{n,n-1}^{(L)} \left(\mathbb{R}_+^{\left[\frac{n-1}{2}\right]+1} \times \Delta_{\left[\frac{n}{2}\right]} \right) \\ & \sqcup \phi_{n,n-1}^{(U)} \left(\mathbb{R}_+^{\left[\frac{n}{2}\right]+1} \times \Delta_{\left[\frac{n-1}{2}\right]} \right), \end{aligned} \quad (3.9)$$

(iii) *when $T = (\infty, \infty)$ and $n = 2m$ is even,*

$$\partial K_n^* = \phi_{n,n-1}^{(L)} \left(\mathbb{R}_+^m \times \Delta_m \right) \quad (3.10)$$

almost surely with respect to the n -dimensional Hausdorff measure, where \sqcup means a disjoint union. The maps $\phi_{n,n-1}^{(U)}$ and $\phi_{n,n-1}^{(L)}$ in (3.9) and (3.10) are diffeomorphic.

Proof. The general forms of the one-to-one representations for $T = [a, b]$, $[a, \infty)$, and $(-\infty, \infty)$ are provided in Section 2 of Chapter II, Section 4 of Chapter V, and Section 5 of Chapter VI, respectively. The last case of $T = (-\infty, \infty)$ is stated in terms of periodic functions. Picking up the terms whose images are n -dimensional, we have (3.9) and (3.10). The second component in (3.9) disappears in (3.10) because when $T = (-\infty, \infty)$ and $n = 2m$, $\psi_n(a) = \psi_n(b) = (0, \dots, 0, 1)^\top$. \square

The following two propositions give representations for the positive polynomial cone K_n and its boundary ∂K_n .

Proposition 3.3. *The positive polynomial cone K_n has the following almost sure representation:*

$$K_n = \varphi_n(\mathbb{R}_+^2 \times \Delta_{n-1})$$

almost surely with respect to the $(n+1)$ -dimensional Lebesgue measure. Here, the function $\varphi_n(\alpha, \gamma) \in \mathbb{R}^{n+1}$ with $\alpha = (\alpha_1, \alpha_2) \in \mathbb{R}_+^2$ and $\gamma = (\gamma_1, \dots, \gamma_{n-1}) \in \Delta_{n-1}$ is the coefficient vector of the polynomial $p_n(t; \alpha, \gamma) = \varphi_n(\alpha, \gamma)^\top \psi_n(t)$ in t defined below:

(i) When $T = [a, b]$,

$$p_n(t; \alpha, \gamma) = \begin{cases} \alpha_1 \prod_{j=1}^m (t - \gamma_{2j-1})^2 + \alpha_2 (t - a)(b - t) \prod_{j=1}^{m-1} (t - \gamma_{2j})^2 & (n = 2m), \\ \alpha_1 (t - a) \prod_{j=1}^m (t - \gamma_{2j})^2 + \alpha_2 (b - t) \prod_{j=1}^m (t - \gamma_{2j-1})^2 & (n = 2m + 1), \end{cases}$$

(ii) when $T = [a, \infty)$,

$$p_n(t; \alpha, \gamma) = \begin{cases} \alpha_1 \prod_{j=1}^m (t - \gamma_{2j-1})^2 + \alpha_2 (t - a) \prod_{j=1}^{m-1} (t - \gamma_{2j})^2 & (n = 2m), \\ \alpha_1 (t - a) \prod_{j=1}^m (t - \gamma_{2j})^2 + \alpha_2 \prod_{j=1}^m (t - \gamma_{2j-1})^2 & (n = 2m + 1), \end{cases}$$

(iii) when $T = (-\infty, \infty)$ and $n = 2m$,

$$p_n(t; \alpha, \gamma) = \alpha_1 \prod_{j=1}^m (t - \gamma_{2j-1})^2 + \alpha_2 \prod_{j=1}^{m-1} (t - \gamma_{2j})^2.$$

The map φ_n is a diffeomorphism. Here, we use the convention $\prod_{j=1}^0 = 1$.

Proof. The representations of the positive polynomials on $T = [a, b]$, $[a, \infty)$, and $(-\infty, \infty)$ whose orders are exactly n are provided in Section 10 of Chapter II, Section 9 of Chapter V, and Section 9 of Chapter VI of Karlin and Studden (1966), respectively. They are unique representations when $\alpha_1 > 0$ and $\alpha_2 > 0$.

Because the contributions of the positive polynomials of order n with $\alpha_1 = 0$ or $\alpha_2 = 0$ and the positive polynomials of order less than n are n -dimensional at most, we do not need to take them into account.

The uniqueness of the representation of p_n implies that the map φ_n is one-to-one. It is obviously differentiable and hence diffeomorphic. \square

Proposition 3.4. *Suppose that $n \geq 2$. The boundary of the positive polynomial cone ∂K_n has the almost sure representation below. Define the functions $\varphi_n^{(i)}(\alpha, \gamma, \tilde{\gamma}) \in \mathbb{R}^{n+1}$ with $n - i \geq 1$, $\alpha \in \mathbb{R}_+^2$, $\gamma \in \Delta_{n-1-i}$, and $\tilde{\gamma} \in \mathbb{R}$, by the coefficient vectors of polynomials as*

$$(t - \tilde{\gamma})^i p_{n-i}(t; \alpha, \gamma) = \varphi_n^{(i)}(\alpha, \gamma, \tilde{\gamma})^\top \psi_n(t) \quad (i = 1, 2).$$

Define the function $\varphi_2^{(2)}(\alpha_1, \tilde{\gamma}) \in \mathbb{R}^3$ with $\alpha_1 \in \mathbb{R}_+$ and $\tilde{\gamma} \in \mathbb{R}$ by the coefficient vector of a polynomial as

$$(t - \tilde{\gamma})^2 \times \alpha_1 = \varphi_2^{(2)}(\alpha_1, \tilde{\gamma})^\top \psi_2(t).$$

(i) When $T = [a, b]$,

$$\begin{aligned} \partial K_n = & \begin{cases} \varphi_n^{(2)}(\mathbb{R}_+^2 \times \Delta_{n-3} \times T) & (n \geq 3), \\ \varphi_2^{(2)}(\mathbb{R}_+ \times T) & (n = 2) \end{cases} \\ & \sqcup \varphi_n^{(1)}(\mathbb{R}_+^2 \times \Delta_{n-2}, a) \\ & \sqcup \left\{ -\varphi_n^{(1)}(\mathbb{R}_+^2 \times \Delta_{n-2}, b) \right\}, \end{aligned} \quad (3.11)$$

(ii) when $T = [a, \infty)$,

$$\begin{aligned} \partial K_n = & \begin{cases} \varphi_n^{(2)}(\mathbb{R}_+^2 \times \Delta_{n-3} \times T) & (n \geq 3), \\ \varphi_2^{(2)}(\mathbb{R}_+ \times T) & (n = 2) \end{cases} \\ & \sqcup \varphi_n^{(1)}(\mathbb{R}_+^2 \times \Delta_{n-2}, a) \\ & \sqcup \varphi_{n-1}(\mathbb{R}_+^2 \times \Delta_{n-2}), \end{aligned} \quad (3.12)$$

(iii) when $T = (-\infty, \infty)$ and $n = 2m$ is even,

$$\partial K_n = \begin{cases} \varphi_n^{(2)}(\mathbb{R}_+^2 \times \Delta_{n-3} \times T) & (n \geq 3), \\ \varphi_2^{(2)}(\mathbb{R}_+ \times T) & (n = 2) \end{cases} \quad (3.13)$$

almost surely with respect to the n -dimensional Hausdorff measure, where \sqcup means a disjoint union. The maps φ_n , $\varphi_n^{(1)}(\cdot, a)$, $\varphi_n^{(1)}(\cdot, b)$, and $\varphi_n^{(2)}$ are diffeomorphisms.

Proof. (i) The case of $T = [a, b]$. The boundary of the positive polynomial cone K_n is proved to consist of the positive polynomials of order n (at most) that have zeros on T . For the almost sure representation, we need only polynomials

of the highest degree. Hence, we can consider only the following three types: $(t - \tilde{\gamma})^2 p_{n-2}(t; \alpha, \gamma)$ ($\tilde{\gamma} \in \text{int } T$), $(t - a)p_{n-1}(t; \alpha, \gamma)$, and $(b - t)p_{n-1}(t; \alpha, \gamma)$ with $\alpha_1, \alpha_2 > 0$. The above three types have no intersection, and (3.11) follows.

(ii) The case of $T = [a, \infty)$. The boundary of the positive polynomial cone K_n is proved to consist of the positive polynomials of order n (at most) that have zeros on T and the positive polynomials of order $n - 1$ (at most). For the almost sure representation, we can consider only the following three types: $(t - \tilde{\gamma})^2 p_{n-2}(t; \alpha, \gamma)$ ($\tilde{\gamma} \in \text{int } T$), $(t - a)p_{n-1}(t; \alpha, \gamma)$, and $p_{n-1}(t; \alpha, \gamma)$ with $\alpha_1, \alpha_2 > 0$. These three types have no intersection, and (3.12) follows.

(iii) The case of $T = (-\infty, \infty)$. The boundary of the positive polynomial cone K_n is proved to consist of the positive polynomials of order n (at most) that have zeros on T and the positive polynomials of order $n - 2$ (at most). For the almost sure representation, we can consider only the case $(t - \tilde{\gamma})^2 p_{n-2}(t; \alpha, \gamma)$ ($\tilde{\gamma} \in T$), and (3.13) follows. \square

3.3 Volume formulas and the weights

The diffeomorphic maps appearing in Propositions 3.1–3.4 are homogeneous functions with respect to their first arguments ρ and α . Therefore, by restricting the length of the first argument, we can construct almost sure representations for the intersections with the unit sphere. For example, $\phi_{n,n}^{(U)}(r\rho, \tau) = r\phi_{n,n}^{(U)}(\rho, \tau)$ for a constant $r > 0$, and we have

$$K_n^* \cap (\mathbb{S}^n)^* = \bar{\phi}_{n,n}^{(U)} \left(\mathbb{S}_+^{\lceil \frac{n+1}{2} \rceil + 1} \times \Delta_{\lfloor \frac{n}{2} \rfloor} \right) \quad \text{a.s.},$$

where

$$\bar{\phi}_{n,l}^{(U)}(\rho, \tau) = \phi_{n,l}^{(U)}(\rho, \tau) / \|\phi_{n,l}^{(U)}(\rho, \tau)\|_{\Sigma},$$

and

$$\mathbb{S}_+^m = \left\{ \rho = (\rho_i) \in \mathbb{R}^{m+1} \mid \sum \rho_i^2 = 1, \rho_i > 0 \right\}. \quad (3.14)$$

Define

$$\begin{aligned} \bar{\phi}_{n,l}^{(L)}(\rho, \tau) &= \phi_{n,l}^{(L)}(\rho, \tau) / \|\phi_{n,l}^{(L)}(\rho, \tau)\|_{\Sigma}, \\ \bar{\varphi}_n(\alpha, \gamma) &= \varphi_n(\alpha, \gamma) / \|\varphi_n(\alpha, \gamma)\|_{\Sigma^{-1}}, \\ \bar{\varphi}_n^{(i)}(\alpha, \gamma, \tilde{\gamma}) &= \varphi_n^{(i)}(\alpha, \gamma, \tilde{\gamma}) / \|\varphi_n^{(i)}(\alpha, \gamma, \tilde{\gamma})\|_{\Sigma^{-1}} \quad (i = 1, 2), \\ \bar{\varphi}_2^{(2)}(\tilde{\gamma}) &= \varphi_2^{(2)}(1, \tilde{\gamma}) / \|\varphi_2^{(2)}(1, \tilde{\gamma})\|_{\Sigma^{-1}} \end{aligned}$$

similarly.

In the proposition below, let $\theta = (\theta_i) \in \Theta_m$ be the local coordinates of \mathbb{S}_+^m in (3.14). For example, $\rho = \rho(\theta) = (\theta_1, \dots, \theta_m, \sqrt{1 - \sum \theta_i^2})$, $\theta \in \Theta_m = \mathbb{R}_+^m$. Another

example is the polar coordinates $\rho(\theta) = (\rho_i(\theta)) \in \Theta_m = (0, \pi/2)^m$ with $\rho_1(\theta) = \cos \theta_1$, $\rho_i(\theta) = \prod_{j=1}^{i-1} \sin \theta_j \cos \theta_i$ ($j = 2, \dots, m$), and $\rho_{m+1}(\theta) = \prod_{j=1}^m \sin \theta_j$.

Proposition 3.5. *Let $\xi = (\theta, \tau)$ and $d\xi = \prod d\theta_i \prod d\tau_i$ be the Lebesgue measure. (ξ may consist of either θ or τ only when the other does not appear in the integrand.) Write $\rho = \rho(\theta)$ for simplicity.*

$$\begin{aligned} \text{Vol}^*(K_n^* \cap (\mathbb{S}^n)^*) &= \int_{\Theta_{[\frac{n+1}{2}]} \times \Delta_{[\frac{n}{2}]}} \det \left\{ \left(\frac{\partial \bar{\phi}_{n,n}^{(U)}(\rho, \tau)}{\partial \xi} \right)^\top \Sigma \left(\frac{\partial \bar{\phi}_{n,n}^{(U)}(\rho, \tau)}{\partial \xi} \right) \right\}^{\frac{1}{2}} d\xi \\ &= \int_{\Theta_{[\frac{n}{2}]} \times \Delta_{[\frac{n+1}{2}]}} \det \left\{ \left(\frac{\partial \bar{\phi}_{n,n}^{(L)}(\rho, \tau)}{\partial \xi} \right)^\top \Sigma \left(\frac{\partial \bar{\phi}_{n,n}^{(L)}(\rho, \tau)}{\partial \xi} \right) \right\}^{\frac{1}{2}} d\xi, \end{aligned}$$

and when $n \geq 2$,

$$\begin{aligned} \text{Vol}^*(\partial K_n^* \cap (\mathbb{S}^n)^*) &= \int_{\Theta_{[\frac{n-1}{2}]} \times \Delta_{[\frac{n}{2}]}} \det \left\{ \left(\frac{\partial \bar{\phi}_{n,n-1}^{(L)}(\rho, \tau)}{\partial \xi} \right)^\top \Sigma \left(\frac{\partial \bar{\phi}_{n,n-1}^{(L)}(\rho, \tau)}{\partial \xi} \right) \right\}^{\frac{1}{2}} d\xi \\ &\quad + \int_{\Theta_{[\frac{n}{2}]} \times \Delta_{[\frac{n-1}{2}]}} \det \left\{ \left(\frac{\partial \bar{\phi}_{n,n-1}^{(U)}(\rho, \tau)}{\partial \xi} \right)^\top \Sigma \left(\frac{\partial \bar{\phi}_{n,n-1}^{(U)}(\rho, \tau)}{\partial \xi} \right) \right\}^{\frac{1}{2}} d\xi \\ &\quad \text{(if } T = [a, b] \text{ or } [a, \infty)). \end{aligned} \quad (3.15)$$

The second term in the right-hand side of (3.15) is not needed when $T = (-\infty, \infty)$.

Proposition 3.6. *Let $\zeta = (\theta, \gamma, \tilde{\gamma})$ and $d\zeta = d\theta \prod d\gamma_i d\tilde{\gamma}$ be the Lebesgue measure. (Some of $\theta, \gamma, \tilde{\gamma}$ may not be included in ζ if they do not appear in the integrand.) Let $\alpha = (\cos \theta, \sin \theta)$.*

$$\text{Vol}(K_n \cap \mathbb{S}^n) = \int_{(0, \frac{\pi}{2}) \times \Delta_{n-1}} \det \left\{ \left(\frac{\partial \bar{\varphi}_n(\alpha, \gamma)}{\partial \zeta} \right)^\top \Sigma^{-1} \left(\frac{\partial \bar{\varphi}_n(\alpha, \gamma)}{\partial \zeta} \right) \right\}^{\frac{1}{2}} d\zeta,$$

and when $n \geq 2$,

$$\begin{aligned}
& \text{Vol}(\partial K_n \cap \mathbb{S}^n) \\
&= \begin{cases} \int_{(0, \frac{\pi}{2}) \times \Delta_{n-3} \times T} \det \left\{ \left(\frac{\partial \bar{\varphi}_n^{(2)}(\alpha, \gamma, \tilde{\gamma})}{\partial \zeta} \right)^\top \Sigma^{-1} \left(\frac{\partial \bar{\varphi}_n^{(2)}(\alpha, \gamma, \tilde{\gamma})}{\partial \zeta} \right) \right\}^{\frac{1}{2}} d\zeta & (n \geq 3), \\ \int_T \left\{ \left(\frac{\partial \bar{\varphi}_2^{(2)}(\tilde{\gamma})}{\partial \tilde{\gamma}} \right)^\top \Sigma^{-1} \left(\frac{\partial \bar{\varphi}_2^{(2)}(\tilde{\gamma})}{\partial \tilde{\gamma}} \right) \right\}^{\frac{1}{2}} d\tilde{\gamma} & (n = 2) \end{cases} \\
&+ \int_{(0, \frac{\pi}{2}) \times \Delta_{n-2}} \det \left\{ \left(\frac{\partial \bar{\varphi}_n^{(1)}(\alpha, \gamma, a)}{\partial \zeta} \right)^\top \Sigma^{-1} \left(\frac{\partial \bar{\varphi}_n^{(1)}(\alpha, \gamma, a)}{\partial \zeta} \right) \right\}^{\frac{1}{2}} d\zeta \\
&\quad \text{(if } T = [a, b] \text{ or } [a, \infty)) \\
&+ \int_{(0, \frac{\pi}{2}) \times \Delta_{n-2}} \det \left\{ \left(\frac{\partial \bar{\varphi}_n^{(1)}(\alpha, \gamma, b)}{\partial \zeta} \right)^\top \Sigma^{-1} \left(\frac{\partial \bar{\varphi}_n^{(1)}(\alpha, \gamma, b)}{\partial \zeta} \right) \right\}^{\frac{1}{2}} d\zeta \\
&\quad \text{(if } T = [a, b]) \\
&+ \int_{(0, \frac{\pi}{2}) \times \Delta_{n-2}} \det \left\{ \left(\frac{\partial \bar{\varphi}_{n-1}(\alpha, \gamma)}{\partial \zeta} \right)^\top \Sigma^{-1} \left(\frac{\partial \bar{\varphi}_{n-1}(\alpha, \gamma)}{\partial \zeta} \right) \right\}^{\frac{1}{2}} d\zeta \\
&\quad \text{(if } T = [a, \infty)). \tag{3.16}
\end{aligned}$$

In the right-hand side of (3.16), the second term is not needed for $T = (-\infty, \infty)$, the third term is not needed for $T = [a, \infty)$ and $(-\infty, \infty)$, the fourth term is not needed for $T = [a, b]$ and $(-\infty, \infty)$.

Substituting the volumes obtained in Propositions 3.5 and 3.6 into (3.3), we get w_{n+1} , w_n , w_0 , and w_1 . Combined with the Gauss-Bonnet theorem (3.4), all weights $\{w_i\}$ for $n \leq 4$ are obtained as follows.

$$(w_0, \dots, w_{n+1}) = \begin{cases} (w_0, \frac{1}{2}, \frac{1}{2} - w_0) = (\frac{1}{2} - w_{n+1}, \frac{1}{2}, w_{n+1}) & (n = 1), \\ (\frac{1}{2} - w_n, w_1, w_n, \frac{1}{2} - w_1) & (n = 2), \\ (w_0, w_1, \frac{1}{2} - w_0 - w_{n+1}, w_n, w_{n+1}) & (n = 3), \\ (w_0, w_1, \frac{1}{2} - w_0 - w_n, \frac{1}{2} - w_1 - w_{n+1}, w_n, w_{n+1}) & (n = 4). \end{cases}$$

For $n > 4$, some of the weights are undetermined. However, thanks to the Gauss-Bonnet theorem (3.4), and noting that $\bar{G}_i(a)$ and $\bar{B}_{\frac{i}{2}, \frac{n+1-i+\nu}{2}}(a)$ are increasing in i , and that $\bar{G}_{n+1-i}(b)$ and $\bar{B}_{\frac{n+1-i}{2}, \frac{\nu}{2}}(b)$ are decreasing in i , we have upper and lower bounds for the marginal distributions of (3.1) and (3.2). For

example, the bounds for λ_{01} and λ_{12} are given by

$$\begin{aligned} \sum_{i=0}^{n+1} u_i \bar{G}_i(a) &\leq P_{H_0}(\lambda_{01} \geq a) \leq \sum_{i=0}^{n+1} v_i \bar{G}_i(a), \\ \sum_{i=0}^{n+1} v_i \bar{G}_{n+1-i}(a) &\leq P_{H_0}(\lambda_{12} \geq a) \leq \sum_{i=0}^{n+1} u_i \bar{G}_{n+1-i}(a), \end{aligned}$$

where

$$\begin{aligned} &(u_0, \dots, u_{n+1}) \\ &= \begin{cases} (w_0, w_1, \frac{1}{2} - w_0 - w_{n+1}, \frac{1}{2} - w_1 - w_n, \underbrace{0, \dots, 0}_{n-4}, w_n, w_{n+1}) & (n : \text{odd}), \\ (w_0, w_1, \frac{1}{2} - w_0 - w_n, \frac{1}{2} - w_1 - w_{n+1}, \underbrace{0, \dots, 0}_{n-4}, w_n, w_{n+1}) & (n : \text{even}), \end{cases} \\ &(v_0, \dots, v_{n+1}) \\ &= \begin{cases} (w_0, w_1, \underbrace{0, \dots, 0}_{n-4}, \frac{1}{2} - w_1 - w_n, \frac{1}{2} - w_0 - w_{n+1}, w_n, w_{n+1}) & (n : \text{odd}), \\ (w_0, w_1, \underbrace{0, \dots, 0}_{n-4}, \frac{1}{2} - w_0 - w_n, \frac{1}{2} - w_1 - w_{n+1}, w_n, w_{n+1}) & (n : \text{even}). \end{cases} \end{aligned}$$

Moreover, since $\bar{G}_i(a) = o(\bar{G}_{n+1}(a))$ as $a \rightarrow \infty$ for $i < n+1$, the tail probabilities of λ_{01} and λ_{12} have asymptotic expressions

$$P_{H_0}(\lambda_{01} \geq a) \sim w_{n+1} \bar{G}_{n+1}(a), \quad P_{H_0}(\lambda_{12} \geq a) \sim w_0 \bar{G}_{n+1}(a)$$

as $a \rightarrow \infty$.

4 Computational aspects

4.1 A numerical procedure for MLE

To obtain the LRT statistics λ_{01} and λ_{12} in (2.1), we need to perform the orthogonal projection onto the positive polynomial cone K . For this purpose, the following symmetric cone programming technique is useful. In this subsection, we treat only the case of $T = [a, b]$ with finite a, b . However, the technique explained here is easily extended to the other cases.

The positive polynomial $p_n(t)$ of degree n on the set T is characterized in Proposition 3.3. This is a unique representation. Admitting the redundancy of

the parameters, this polynomial is rewritten as

$$p_n(t) = \begin{cases} \psi_m(t)^\top Q_1 \psi_m(t) + (t-a)(b-t) \psi_{m-1}(t)^\top Q_2 \psi_{m-1}(t) & (n = 2m), \\ (t-a) \psi_m(t)^\top Q_1 \psi_m(t) + (b-t) \psi_m(t)^\top Q_2 \psi_m(t) & (n = 2m+1), \end{cases} \quad (4.1)$$

where Q_1 and Q_2 are symmetric positive semi-definite matrices. This polynomial (4.1) is obviously nonnegative on $T = [a, b]$. Conversely, the polynomial $p_n(t)$ in Proposition 3.3 can be written as (4.1). This representation is sometimes referred to as the Markov-Lukacs theorem (Nesterov (2000)).

By arranging the terms, the polynomial $p_n(t)$ in (4.1) can be written as $p_n(t) = e(Q_1, Q_2)^\top \psi_n(t)$, where $e(Q_1, Q_2)$ is a $(n+1)$ -dimensional column vector depending on Q_1 and Q_2 . Using this representation, the orthogonal projection of a given vector \hat{c} onto the positive polynomial cone K is formalized as the optimization problem below:

$$\begin{aligned} \text{maximize} \quad & -d \\ \text{subject to} \quad & d \geq \|\hat{c} - c\|_{\Sigma^{-1}} \quad (\text{quadratic cone restriction}) \\ & c = e(Q_1, Q_2) \quad (\text{linear restriction}) \\ & Q_1, Q_2 \succeq 0 \quad (\text{PSD cone restriction}) \end{aligned}$$

This is an optimization problem with quadratic cone, linear, and positive semi-definite (PSD) cone restrictions. This can be solved in the framework of symmetric cone programming. Several public softwares are available (e.g., SeDuMi by Sturm (1999)).

Figure 4.1 shows an example of orthogonal projection. Let K be the positive polynomial cone of order $n = 3$ on the set $T = [a, b] = [0, 1]$. Under the metric $\|\cdot\|_{\Sigma^{-1}}$ with $\Sigma = ((i+j-1)^{-1})_{1 \leq i, j \leq 4}^{-1}$, the orthogonal projection of $f(t; \hat{c}) = 0.5t - 1.5t^2 + t^3$ onto K is given by $f(t; \hat{c}_K) = 0.0258 + 0.5151t - 1.4891t^2 + 1.0086t^3$. In Figure 4.1, $f(t; \hat{c})$ is depicted as a dashed line (- - -), and the projection $f(t; \hat{c}_K)$ is depicted as a solid line (—).

4.2 Analysis of growth curve data: An example

In this subsection, we analyze growth curve data cited in Potthoff and Roy (1964). The dataset consists of a certain measurement on dental study for 11 girls and 16 boys at ages 8, 10, 12, and 14 years.

In our study, let t be the age minus 11 for stabilizing numerical calculations. The measurements of the individual h at the age $t + 11$ in the girl and boy groups

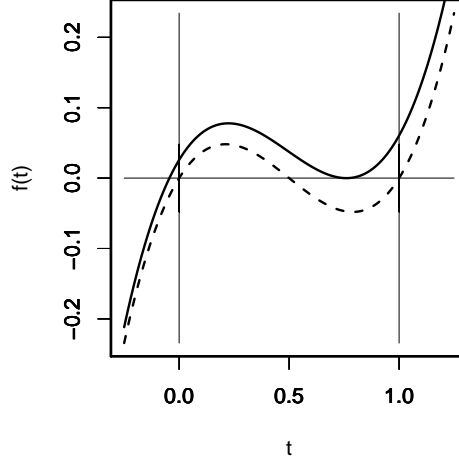


Figure 4.1: Projection onto the positive polynomial cone K_3 .

are denoted by x_{0ht} and x_{1ht} , respectively. For modeling the difference of the profiles (mean vectors) of two groups, we assume the multivariate normal model:

$$\begin{aligned} x_{0ht} &= \mu_t + \varepsilon_{0th}, \quad h = 1, \dots, n_0 (= 11), \\ x_{1ht} &= \mu_t + f(t; c) + \varepsilon_{1th}, \quad h = 1, \dots, n_1 (= 16), \end{aligned} \quad (4.2)$$

with

$$f(t; c) = c_0 + c_1 t + c_2 t^2 + c_3 t^3,$$

where $\varepsilon_{jh} = (\varepsilon_{jht})_{t \in \{-3, -1, 1, 3\}}$ ($j = 0, 1$) are independent Gaussian error vectors with mean zero. For the covariance matrices, we assume the intraclass correlation structure

$$\Sigma_j = \text{Cov}(\varepsilon_{jh}, \varepsilon_{jh}) = \tau_j \{(1 - \rho_j)I + \rho_j J\} \quad (j = 0, 1), \quad (4.3)$$

where J is the 4×4 matrix with all entries 1, and τ_j and ρ_j are unknown parameters. The model (4.3) is widely used covariance structure in the analysis of growth curves and repeated measurements (Crowder and Hand (1990), Kato, Yamada and Fujikoshi (2010)).

Under the model (4.2) with (4.3), the MLEs are calculated as

$$\hat{c} = (\hat{c}_0, \hat{c}_1, \hat{c}_2, \hat{c}_3)^\top = (2.053, 0.551, 0.0536, -0.0301)^\top,$$

and $\hat{\tau}_0 = 4.469$, $\hat{\rho}_0 = 0.868$, $\hat{\tau}_1 = 5.147$, $\hat{\rho}_1 = 0.479$. If Σ_0 and Σ_1 are known, \hat{c} is distributed as the normal distribution with covariance matrix $\Sigma = (F^\top V^{-1} F)^{-1}$, where $V = n_0^{-1} \Sigma_0 + n_1^{-1} \Sigma_1$ and $F = (t^i)_{t \in \{-3, -1, 1, 3\}, 0 \leq i \leq 3}$ is the design matrix. The

MLE of Σ is obtained as

$$\hat{\Sigma} = \begin{pmatrix} 0.649 & 0 & -0.0173 & 0 \\ 0 & 0.140 & 0 & -0.0157 \\ -0.0173 & 0 & 0.00345 & 0 \\ 0 & -0.0157 & 0 & 0.00192 \end{pmatrix}$$

In the following, we treat $\hat{\Sigma}$ as the true value, and suppose the statistics \hat{c} to be a Gaussian vector with mean c and covariance matrix $\hat{\Sigma}$ as an approximating analysis.

Let us focus on the whole period from ages 8 to 14 years, that is, $T = [-3, 3]$, and consider the positivity on the set T . The hierarchical hypotheses in (1.4) are $H_0: f(t; c) \equiv 0$ ($c = 0$), $H_1: f(t; c)$ is a positive polynomial on T ($c \in K$), and $H_2: f(t; c)$ is unrestricted ($c \in \mathbb{R}^4$). Since $f(t; \hat{c})$ is already positive on T , the orthogonal projection \hat{c}_K is \hat{c} itself, and the LRT statistic for testing H_0 against H_1 is $\lambda_{01} = \|\hat{c}_K\|_{\hat{\Sigma}^{-1}}^2 = \|\hat{c}\|_{\hat{\Sigma}^{-1}}^2 = 19.293$. This looks highly significant because the p -value referring to the chi-square distribution with 4 degrees of freedom is already 0.000688. Actually, by means of Propositions 3.5 and 3.6, the weights for the distribution of λ_{01} are

$$(w_0, w_1, w_2, w_3, w_4) = (0.0072, 0.0657, 0.2416, 0.4343, 0.2512),$$

and the p -value for λ_{01} is obtained as 0.000293. We conclude that the growth curve of the boy group is always beyond that of the girl group.

Then, what about the growth rates of two groups. Is the growth rate of the boy group always greater than that of the girl group? In order to confirm this hypothesis, let us take the differential of $f(t; \hat{c})$:

$$f'(t; \hat{c}) = \hat{c}_1 + 2\hat{c}_2 t + 3\hat{c}_3 t^2 = f(t; \hat{d}),$$

where

$$\hat{d} = L\hat{c} = (0.551, 0.107, -0.0902)^\top, \quad L = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix}.$$

We suppose that \hat{d} is distributed as the normal distribution $N_3(d, L\hat{\Sigma}L^\top)$, $d = Lc$. Here again, we consider the hierarchical hypotheses in (1.4) that $H_0: f'(t; c) \equiv 0$ ($d = 0$), $H_1: f'(t; c)$ is a positive polynomial on T ($d \in K$), and $H_2: f'(t; c)$ is unrestricted ($d \in \mathbb{R}^3$). Since $f'(-3; \hat{c}) = -0.582 < 0 < f'(0; \hat{c}) = \hat{c}_1$, $f'(t; \hat{c})$ is not a positive polynomial on $T = [-3, 3]$. The orthogonal projection of \hat{d} onto K under the metric $\langle \cdot, \cdot \rangle_{(L\hat{\Sigma}L^\top)^{-1}}$ is

$$\hat{d}_K = (0.348, 0.0776, -0.0128)^\top.$$

The LRT statistics for testing H_0 against H_1 , and for testing H_1 against H_2 are obtained as $\lambda_{01} = 9.293$ and $\lambda_{12} = 0.417$, respectively. The weights are computed as

$$(w_0, w_1, w_2, w_3) = (0.3318, 0.4792, 0.168, 0.0208).$$

Using these weights, the p -values for λ_{01} and λ_{12} are calculated as 0.00324 and 0.787, respectively. Thus, the hypothesis that f' is a positive polynomial is accepted, and the hypothesis that $f' \equiv 0$ is rejected at the 1% significance level. We conclude that the growth rate of the boy group is always greater than that of the girl group between the age 8 and 14.

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